IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	Crystal Plasticity Modeling of Mg	
Project Number	**IMURA1066**	
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Research Clusters:

Research Themes:

Highlight which of the Academy's CLUSTERS this project will address?
***(**Please nominate JUST **one.** For more information, see www.iitbmonash.org)*

1.Material Science/Engineering (including Nano, Metallurgy)
2.Energy, Green Chem, Chemistry, Catalysis, Reaction Eng
3.Math, CFD, Modelling, Manufacturing
4.CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control
5.Earth Sciences and Civil Engineering (Geo, Water, Climate)
6.Bio, Stem Cells, Bio Chem, Pharma, Food
7.Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng
8.HSS, Design, Management

Highlight which of the Academy's Theme(s) this project will address?
(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1.Advanced computational engineering, simulation and manufacture
2.Infrastructure Engineering
3.Clean Energy
4.Water
5.Nanotechnology
6.Biotechnology and Stem Cell Research
7.Humanities and social sciences
8.Design

The research problem

Mg is increasingly seen as a key component for lightweight structures and bio-implants. Due to hexagonal crystal structure, deformation by dislocation slip is difficult in Mg and its alloys. Twinning is a key deformation mode in Mg. Past studies show that twinning in Mg is dependent on a number of factors e.g. deformation conditions, number of twins per twinned grain, grain area. Apart from these, grain boundary characteristics play an important role on twin nucleation.

This project focuses on development of a crystal plasticity model that can address complex twinning mechanisms and slip-twin interactions in Mg and its alloys. Current crystal plasticity models assume accumulated slip system activity to be the deciding factor for twin nucleation. However, such models are not fully predictive. Thus, we intend to focus on local prevailing conditions e.g. grain boundaries for establishing laws of twin nucleation and growth in Mg.

Crystal plasticity models are built upon concepts of continuum mechanics and physics of plasticity. A mathematical framework addressing micromechanisms of plastic deformations is solved in conjunction with the conservation of laws of mechanics and thermodynamics. The set of equations are solved using numerical methods e.g. finite element method.

For calibrating the model, mechanical characterization and microstructure characterization (using EBSD, TEM) will be performed.

A few examples of relevant reading are as following:

1. Nie et al., Periodic segregation of solute atoms in fully coherent twin boundaries, Science, 340, 2013, p. 957
2. Gong et al., Symmetric or asymmetric glide resistance to twinning disconnection?, npj Computational Materials, 2022.
3. Dadhich and Alankar, A modular spectral solver for crystal plasticity, International Journal of Plasticity, 2022, p. 103328.
4. Dhala et al., Modeling of finite deformation of pseudoelastic NiTi shape memory alloy considering various inelasticity mechanisms, International Journal of Plasticity, 2019, p. 216.

Project aims

1. Mechanical characterization of Mg at room temperature.
2. Understanding twinning behaviour with help of EBSD and TEM.
   Incorporation of twinning mechanisms in crystal plasticity.
   Advanced simulations for validation.

Expected outcomes

1. A robust understanding of mechanical behavior of Mg and role of various mechanisms of twinning.
2. Dataset of structure-process-property
3. A crystal plasticity model for Mg which will be extendible to other hexagonal metals as well.
   Understanding on process route for application in automotive industry

How will the project address the Goals of the above Themes?

The objective of this project is to understand fundamental mechanisms of twinning in Mg. After investigating such mechanisms via experiments these will be incorporated in a crystal plasticity based deformation model using finite element method. Such models are predictive in nature and will be helpful in understanding deformation at arbitrary mechanical conditions. This project involves concepts of metallurgical engineering and computational mechanics.

Capabilities and Degrees Required

List the ideal set of capabilities:

1. Plasticity
2. Crystal Plasticity
3. Mechanics of Materials
4. Numerical Methods e.g. finite element method
5. Programming in C++ or FORTRAN or Python

Potential Collaborators

DBT, General Electric, ISRO, BARC,CSIRO. We have not contacted any yet.